On Bose-Einstein condensation in quasi-2D systems with applications to high T_c superconductivity II.

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(Dated: December 9, 2009)

We calculate the number and energy densities of a quasi-2D Bose-Einstein gas constrained within a thin region of infinite extent but of finite width δ. The BEC critical transition temperature then becomes an explicit function of δ. We use this result to construct a model of high-T_c superconductivity in cuprates with a periodic layered atomic structure. The predicted behavior of the BEC T_c agrees with recent experimental findings in severely underdoped cuprates.

PACS numbers: 05.30.Fk, 74.20.-z, 74.72.-h

INTRODUCTION

Since the discovery of high-T_c superconductivity (HTSC) in cuprates by Bednorz and Müller in 1986 many studies to explain the phenomenon have been reported. Its physical origin is not yet clear. Recent measurements [1] of photoelectron emission spectral intensities from HTSCs suggest that bound electron Cooper pairs (CPs) form already at temperatures higher than the critical T_c. This finding is consistent with several theoretical efforts [3, 4] proposing that HTSC originates from a 2D Bose-Einstein condensate (BEC) of CPs pre-existing above T_c and formed through a BCS-like phonon mechanism. The 2D character of the phase transition is associated with the layered structure of cuprates, which in the case of $YBa_2Cu_3O_{7-y}$ (YBCO) consists of a succession of parallel layers perpendicular to the vertical c-axis with a unit cell of height $\sim 12\mathring{A}$, and the chemical composition $CuO-BaO-CuO_2-Y-CuO_2-BaO-CuO$. It is generally agreed that the CuO_2 planes, which in the case of YBCO are equidistant from the central Y atom with separation $\simeq 1.5\mathring{A}$, are mainly responsible for the superconductivity in cuprates. Contour plots of the charge distribution derived from energy-band-structure calculations for YBCO reveal [5] that the SC charge carriers are mainly concentrated within a slab of width $\delta \simeq 2.15\mathring{A}$ about the CuO_2 plane.

BCS-like theories [3, 4] contemplate a Hamiltonian H_{BCS} containing the kinetic energies of electrons and holes, and a pairing interaction arising from phonon-exchange attractions that overwhelm and Coulombic repulsion. As a consequence, bound CPs of electrons or holes with antiparallel spins and charge $\pm 2e$ arise with an energy-momentum relation linear at leading order, rather than quadratic, namely $\mathcal{E}_K \simeq \mathcal{E}_0 + c_1\hbar K$ with $c_1 = 2v_F/\pi$ in 2D with v_F the Fermi speed, while K is the CP center-of-mass momentum wavenumber, and $\mathcal{E}_0$ the familiar weak-coupling energy $\mathcal{E}_0 = -2\hbar\omega_D \exp[-2/v_0N_0]$ for $K = 0$ CPs, where ω_D is the Debye frequency, v_0 the positive BCS electron-phonon coupling constant, and N_0 the electron density of states for one spin at the Fermi level. The linear dispersion relation is induced [2] by the Fermi sea medium so that CPs propagate like free massless composite particles in the Fermi sea (whereas *in vacuo* they would do so quadratically as $\hbar^2K^2/4m^*$ if m^* is the effective electron mass). Their Bose statistical nature allows them to undergo BEC.

FORMALISM

We study a model of HTSC in cuprate materials comprising a quasi-2D BEC of excited CPs of energy $\mathcal{E}_K \simeq \mathcal{E}_0 + c_1\hbar K$ constrained to propagate within quasi-2D layers of infinite extent in the a_1, a_2 directions, but of finite width $a_3 = \delta$ in the perpendicular direction. We assume that the CP field satisfies periodic boundary conditions (BC) along the a_1, a_2 and a_3 directions, although the more restrictive Dirichlet or Neumann BCs may be straightforwardly implemented. The average number density and the energy per unit volume of the CP field are given by

$$n(T) = \frac{1}{V}\int dK \frac{g(K)}{e^{\beta(\varepsilon_K-\mu)}-1} \quad \text{and} \quad u(T) = \frac{1}{V}\int dK \frac{g(K)\varepsilon_K}{e^{\beta(\varepsilon_K-\mu)}-1} \tag{1}$$

where $g(K)$ is the *exact* eigenmode distribution of the field defined by $g(K) = \sum_{\{\mathbf{n}\}} \delta(K - K_{\mathbf{n}})$ with $K^2_{\mathbf{n}} = (2n_1\pi/a_1)^2 + (2n_2\pi/a_2)^2 + (2n_3\pi/a_3)^2$. By introducing Poisson's summation formula it may be shown that $g(K)$ can be expressed

in the more tractable way

$$g(K)=\frac{V}{2\pi^2}K\sum_{m_1,m_2,m_3}\frac{\sin\left[K\left((a_1m_1)^2+(a_2m_2)^2+(a_3m_3)^2\right)^{1/2}\right]}{[(a_1m_1)^2+(a_2m_2)^2+(a_3m_3)^2]^{1/2}}. \tag{2}$$

An alternative derivation based on properties of Bessel functions has been formerly employed to study the Casimir energy-momentum tensor in rectangular cavities, both at zero and finite temperatures [6]. We then evaluate (1) by introducing the CP mode distribution (2) and the CP excitation energy $\varepsilon_K \equiv \mathcal{E}_K - \mathcal{E}_0 \simeq c_1\hbar K$. The Bose-Einstein denominators in the integrals render a rapid convergence so that they may safely be extended to infinity. The integrals can be computed by expanding the integrand in powers of ze^{-x} with the result

$$n(T)=n_0(T)+\frac{(k_BT)^3}{\pi^2\hbar^2c^3}\sum_{m_1,m_2,m_3}\sum_{m=1}^{\infty}\frac{m\ z^m}{\left(m^2+\alpha^2_{m_1,m_2,m_3}\right)^2} \tag{3}$$

with $\alpha^2_{m1,m2,m3}=(k_BT/\hbar c_1)^2[(m_1a_1)^2+(m_2a_2)^2+(m_3a_3]^2$ while the energy density is

$$u(T)=\frac{(k_BT)^4}{\pi^2\hbar^2c_1^3}\sum_{m_1,m_2,m_3}\sum_{m=1}^{\infty}\frac{\left(3m^2-\alpha^2_{m_1,m_2,m_3}\right)z^m}{\left(m^2+\alpha^2_{m_1,m_2,m_3}\right)^3}. \tag{4}$$

It is easily checked that the usual thermodynamic limit is attained by considering the terms with $m_1=m_2=m_3=0$ in the former expressions. On the other hand, for CPs constrained to move within a layer of finite width $\delta \ll a_1, a_2$ but unconstrained along the infinite a_1, a_2 directions we must set $m_1=m_2=0$ in(3) and (4). In that case, we introduce the dimensionless thickness variable $\eta \equiv k_BT\delta/\hbar c_1$ and the remaining summations over m_3 may be performed analytically to give

$$n(T)=n_0(T)+\frac{(k_BT)^3}{\pi^2\hbar^3c^3}\Psi_3(z,\eta)\quad\text{and}\quad u(T)=3\frac{(k_BT)^4}{\pi^2\hbar^3c^3}\Phi_4(z,\eta) \tag{5}$$

where $\Psi_s(z,\eta)\equiv\sum_{m=1}^{\infty}\frac{z^m}{m^s}f_m(\eta)$ and $\Phi_s(z,\eta)\equiv\sum_{m=1}^{\infty}\frac{z^m}{m^s}g_m(\eta)$ with $f_m(\eta)=\frac{1}{2}\left[h_m(\eta)+\frac{m\pi}{\eta}\coth\left(\frac{m\pi}{\eta}\right)\right]$, $h_m(\eta)=\left(\frac{m\pi}{\eta}\right)^2\sinh^{-2}\left(\frac{m\pi}{\eta}\right)$, and $g_m(\eta)=\frac{1}{3}\left[\left(h_m(\eta)+\left(\frac{m\pi}{\eta}\right)\coth\left(\frac{m\pi}{\eta}\right)(1+h_m(\eta)\right)\right]$.

THICK- AND THIN-LAYER LIMITS

The thick-layer limit given by $\eta \gg 1$ represents unconstrained propagation of CPs throughout the entire volume of the material as in conventional 3D superconductivity. In this limit $h_m(\eta)\to 1$, $f_m(\eta)\to 1$, $g_m(\eta)\to 1$ and we recover well-known expressions describing 3D BECs [3, 4]:

$$n(T)=n_0(T)+\frac{(k_BT)^3}{\pi^2\hbar^3c^3}\sum_{m=1}^{\infty}\frac{z^3}{m^3}\quad\text{and}\quad u(T)=3\frac{(k_BT)^4}{\pi^2\hbar^3c^3}\sum_{m=1}^{\infty}\frac{z^4}{m^4} \tag{6}$$

The critical temperature T_c follows from the conditions $n_0(T_c)\to 0$ and $z(T_c)\to 1$ leading to $k_BT_c^{3D}=[\pi^2\hbar^3c_1^3n^{3D}/\zeta(3)]^{1/3}$ where $\zeta(n)$ is Riemann's ζ-function. The molar heat capacity $C(T)=R(nk_B)^{-1}\partial u(T)/\partial T$ (with R the gas constant) is straightforwardly obtained from (6) as $C(T)=\left(\frac{12R\zeta(4)}{\zeta(3)}\right)\left(\frac{T}{T_c}\right)^3$ for $T<T_c$ and $C(T)=\left(\frac{12R\zeta(4)}{\zeta(3)}\right)\left(\frac{T}{T_c}\right)^3-\left(\frac{12R\zeta(3)}{\zeta(2)}\right)$ for $T>T_c$ which is consistent with measurements in conventional 3D superconductors [8] since at $T=T_c$ the heat capacity shows a discontinuous drop $\Delta C=6.57R$ indicative of a second-order phase transition.

In the thin-layer limit $\eta \ll 1$ associated with HTSC we get $h_m(\eta)\to 0$, $f_m(\eta)\simeq m\pi/2\eta$, and $g_m(\eta)\simeq m\pi/3\eta$. Simple algebra leads to

$$n^{2D}(T)=n_0^{2D}(T)+\frac{(k_BT)^2}{2\pi\hbar^2c_1^2}\sum_{m=1}^{\infty}\frac{z^m}{m^2}\quad\text{and}\quad u^{2D}(T)=\frac{(k_BT)^3}{\pi\hbar^2c_1^2}\sum_{m=1}^{\infty}\frac{z^m}{m^3}, \tag{7}$$

where $n^{2D} \equiv n\delta$ and $u^{2D} \equiv u\delta$. The critical BEC temperature is now given by $k_B T_c^{2D} = [2\pi\hbar^2 c_1^2 n^{2D}/\zeta(2)]^{1/2}$ where $\zeta(2) = \pi^2/6$. In this case the molar heat capacity is $C(T) = [6R\zeta(3)/\zeta(2)]\,(T/T_c)^2$ for $T < T_c$ but it must be evaluated numerically for $T > T_c$. It turns out that the $C(T)$ is continuous at $T = T_c$ although its derivative $\partial C/\partial T$ is discontinuous. The linear behavior $C(T)/T \propto T$ for $T \leq T_c$ is characteristic of cuprate materials [9].

Of crucial importance in evaluating T_c is to reliably estimate the fraction of charge carriers that actually contribute to the supercurrent. The charge carrier density is usually determined from measurements of London penetration depth λ_{ab} along the CuO_2 planes. It gives an estimate of the supercurrent that causes partial rejection of an applied external magnetic field in the superconductor. Within the framework of the present model the supercurrent is due to massless-like CPs of charge $2e$ moving with the CP speed c_1, so that the surface supercurrent $\mathbf{J}_s = n^{2D}(2e)c_1\hat{\mathbf{k}}$ with $\hat{\mathbf{k}} \equiv \mathbf{k}/k$ [4]. A straightforward calculation [7] shows that $n^{2D} = (e^2/32\pi c_1^2 c^2)\delta\Delta_0^2/\hbar\omega_D\lambda_{ab}^2$ where c is the speed of light and Δ_0 is the zero-temperature energy gap. The final expression of the BEC critical temperature is

$$T_c = \frac{\hbar c}{2\pi k_B e}\left(\frac{3\delta}{2\hbar\omega_D}\right)^{1/2}\frac{\Delta_0}{\lambda_{ab}}. \tag{8}$$

CONCLUSIONS

Introducing in (8) the YBCO parameters tabulated in Ref.[8] $\Theta_D = 410$ K , $\Delta_0 = 14.5$ meV, and $\delta = 2.15$ Å [5] we get the relation $T_c = 16.79/\lambda_{ab}$ (μm-K) which accurately reproduces experimental data reported by Zuev *et al.* [10] in measurements performed in YBCO films with T_cs ranging from 6 to $50K$. They conclude that, within some noise their data fall on the same curve $\lambda_{ab}^{-2} \propto T_c^{2.3\pm0.4}$ regardless of annealing procedure, oxygen content, etc. In an independent study, Broun *et al.* [11] found that their samples of high-purity single-crystal YBCO followed also the rule $T_c \propto \lambda_{ab}^{-1}$. A forthcoming paper [7] gives a more detailed discussion of the model presented here applied also to several other cuprates including the l-wave extension of the present formalism valid only for $l = 0$.

Acknowledgments We thank D.M. Eagles, M. Fortes, S. Fujita and M.A. Solís for fruitful discussions. MdeLl thanks UNAM-DGAPA-PAPIIT (Mexico) IN106908 for partial support and is grateful to W.C. Stwalley for discussions and the University of Connecticut for its hospitality while on sabbatical leave.

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